there is no substantial difference in the results of these two investigations it will suffice to write a note on the difference in method and agreement of the results.

The two simplest crystals used were selected from a group of small intergrown prismatic crystals prepared by the American Electro-Metal Corporation by the electrolysis of fused borate baths. Precession and Weissenberg methods were used and intensities were visually estimated. The following cell dimensions were obtained:

$$a=2{\cdot}96, \quad b=7{\cdot}81 \quad \text{and} \quad c=2{\cdot}94 \text{ A.},$$

which are within 0·6 % of those found by Dr Keissling. The diffraction symbol was determined as *mmmC–c–*. These dimensions and a density of 6·2 g.cm.$^{-3}$ require four CrB molecules per cell, and the symmetry necessitates that all the atoms fall on fourfold special positions with the x parameter fixed at 0 and perhaps the z parameter fixed at 0·25, but with the y parameter to be determined. Taking advantage of the fact that the chromium atoms will dominate the intensities, but accounting for the influence of the boron, the chromium y parameter was determined graphically from the $(0k0)$ reflections of a Weissenberg picture taken with molybdenum radiation on a composite crystal having a common b axis but with the a axis in one part of the crystal coincident with the c axis in the other. In drawing curves representing change of intensity with change in chromium y parameter for each reflection $(0k0)$, areas were plotted whose boundaries were determined by the maximum possible in-phase and out-of-phase scattering of boron for that reflection. The chromium y parameter was observed to be $0{\cdot}146 \pm 0{\cdot}007$, with 0·143 favored from a closer inspection of the relative intensities and from geometrical considerations.

The y parameter of the boron was determined graphically to be $0{\cdot}45 \pm 0{\cdot}03$ from curves showing the variation of boron y parameter with intensity for each reflection $(0k0)$ assuming 1·43 to be the correct chromium parameter. To equate the length of the bonds to the nearest chromium atoms which form a co-planar triangle 0·43 seems the best boron y parameter.

From the intensities of the $(0kl)$ reflections from a zero-level a-axis precession photograph of a crystal twinned with (110) as the twin law, and accounting for the fact that the $(04l)$ and $(08l)$ reflections were superimposed with the $(13l)$ and $(26l)$ reflections respectively, the z parameters for both the chromium and the boron atoms were confirmed to be 0·25, thus placing both the boron and chromium atom in the 4(c) special position of space group $Cmcm$–D_{2h}^{17} (nomenclature that of the *Internationale Tabellen*) with the y parameters as determined above. These parameters are within 2·3 % of those determined by Dr Keissling.

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The space group of calcium peroxide octahydrate.[*]

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Compounds in which eight molecules of water are co-ordinated about a central ion have been studied, but in no instance has an analysis been reported which can be accepted as representing the correct structure.

Natta (1928, 1932) examined the octahydrate of strontium hydroxide[†] by Laue, rotation and powder methods, and the octahydrate of strontium peroxide[‡] by the powder method alone. He proposed structures for these substances in which the water was cubically co-ordinated about the strontium ion. On the basis of powder data, Miller & King (1936) arrived at a similar conclusion for $CaO_2.8H_2O$, $SrO_2.8H_2O$ and $BaO_2.8H_2O$.[§] In all cases the system was found to be tetragonal with a primitive cell containing a single molecule.

Mellor (1938) reinvestigated $Sr(OH)_2.8H_2O$ by single-crystal methods, but he was unsuccessful in determining the atomic positions. He reported the space group to be D_{2h}^{4}–$P4/mmc$, with a cell having the dimensions $a=8{\cdot}97$, $c=11{\cdot}55$ A. which contained four molecules instead of one as reported by Natta (1928).

The alkaline earth metal peroxide octahydrates are quite insoluble in water, hence previous investigations of their structures have been limited to the powder method.

By slow diffusion of NH_3 into a very cold solution containing a mixture of $Ca(NO_3)_2$ and H_2O_2, crystals of $CaO_2.8H_2O$ suitable for single-crystal studies have been obtained. The data presented below represent the preliminary results of a reinvestigation of this compound.

Optical and Laue studies confirmed the tetragonal character of the crystal. Oscillation patterns taken about the a and c axes gave the cell dimensions $a=6{\cdot}21$, $c=11{\cdot}00$ A. The density, 1·672 g.cm.$^{-3}$, obtained by the flotation method, required a cell containing two molecules instead of one, as previously reported. Systematic extinctions occurred only for $(h0l)$, $(00l)$ and (hhl) with l odd, hence the space group is either D_{h}^{2}–$P4/mcc$ or C_{4v}^{5}–$P4cc$. The latter was ruled out as improbable on the basis of the equivalent positions available for the atoms of two molecules of $CaO_2.8H_2O$.

A preliminary attempt to establish the positions of the atoms by trial methods led to inconclusive results, but indicated that the water molecules probably occupy the sixteen general positions of the space group with approxi-

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[†] $Sr(OH)_2.8H_2O$. Tetragonal. $a=6{\cdot}41$, $c=5{\cdot}807$ A. Sr^{++} at 0, 0, 0. (OH)′ at $\frac{1}{2}, 0, 0$; $0, \frac{1}{2}, 0$. H_2O at x, x, z; $x, x, \bar{z}$; $\bar{x}, x, z$; $\bar{x}, x, \bar{z}$; $x, \bar{x}, z$; $x, \bar{x}, \bar{z}$; $\bar{x}, \bar{x}, z$; $\bar{x}, \bar{x}, \bar{z}$; with $x=0{\cdot}29$–$0{\cdot}30$; $z=0{\cdot}25$.

[‡] $SrO_2.8H_2O$. Tetragonal. $a=6{\cdot}32$; $c=5{\cdot}56$ A. Sr^{++} at 0, 0, 0. O′ at $\frac{1}{2}, \frac{1}{2}, \pm z$; with $z=0{\cdot}10$. H_2O at x, x, z; $x, x, \bar{z}$; $\bar{x}, x, z$; $\bar{x}, x, \bar{z}$; $x, \bar{x}, z$; $x, \bar{x}, \bar{z}$; $\bar{x}, \bar{x}, z$; $\bar{x}, \bar{x}, \bar{z}$; with $x=0{\cdot}20$; $z=0{\cdot}25$.

§	a (A.)	c (A.)	w	x	y	z
$CaO_2.8H_2O$	6·20	5·50	0·12	0·32	0·11	0·25
$SrO_2.8H_2O$	6·32	5·55	0·11	0·32	0·13	0·26
$BaO_2.8H_2O$	6·51	5·75	0·10	0·32	0·12	0·27

Sr^{++} at 0, 0, 0. O′ at $\frac{1}{2}, \frac{1}{2}, \pm w$. H_2O at x, y, z; $\bar{x}, \bar{y}, z$; $x, y, \bar{z}$; $\bar{x}, \bar{y}, \bar{z}$; $\bar{y}, x, z$; $y, \bar{x}, z$; $\bar{y}, x, \bar{z}$; $y, \bar{x}, \bar{z}$.

mate parameters $x=0{\cdot}30$, $y=0{\cdot}11$, $z=0{\cdot}13$. Calculated structure amplitudes with Ca^{++} at 0, 0, 0; 0, 0, ½; O′ at ½, ½, $\pm z$ with $z=0{\cdot}06$ and for an arrangement with Ca^{++} at 0, 0, ¼; 0, 0, ¾; O′ at ½, ½, $\pm z$ with $z=0{\cdot}19$ were almost equally in good agreement with observed values. The slight difference in agreement, however, favored the latter positions which place the water molecules at the corners of a square Archimedean antiprism about the calcium ion at the center of the co-ordination group.

This investigation is being continued in an effort to establish the correct structure, and to note the effect on the structure as the radius of the central ion varies in the series $CaO_2.8H_2O$, $SrO_2.8H_2O$ and $BaO_2.8H_2O$.

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The structure of the ferroelectric niobates and tantalates.

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The symmetries and parameters of the recently reported ferroelectric materials $KTaO_3$, $KNbO_3$, $NaTaO_3$, $NaNbO_3$ (Matthias, 1949) have been measured by X-ray powder methods. At room temperature $KTaO_3$ is cubic and the other compounds are orthorhombic in symmetry. $NaNbO_3$ and $KNbO_3$ have tetragonal and cubic phases at higher temperatures similar to $BaTiO_3$, but $NaNbO_3$ has no rhombohedral phase as low as −173° C.

Untwinned crystals of $NaNbO_3$ have been investigated by single-crystal methods. The unit cell has dimensions $\bumpeq 5{\cdot}6\times 16\times 5{\cdot}6$ A. and contains eight molecules. The space group is $P22_12$ and the structure has twenty-six parameters, most of which have been determined. The results show a displacement of the niobium ions by $\approx 0{\cdot}1$ A. along the long orthorhombic axis.

The space group conclusively shows the structure to be non-polar unless the symmetry is really monoclinic (cf. Rochelle salt). However, optical and X-ray measurements have shown that any shear of the faces is $<0{\cdot}1'$, which is $<\frac{1}{300}$ of the orthorhombic distortion. The conclusion that orthorhombic $NaNbO_3$ is non-polar is most unexpected but can thus hardly be avoided.

A consistent explanation of the ion displacements can be given in terms of packing considerations alone. It is supposed that the orthorhombic distortion caused by the ferroelectricity allows ion shifts which reduce the misfit caused by the small sodium ion. It is this arrangement that can be shown to be non-polar. A detailed account of these researches will be published later.

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Crystal structure of 2,5-dimethoxy-2,5-dimethyl-1,4-dioxane.*

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This compound was of interest to us because of a report by Bergmann (1924) that it forms a crystalline iodine addition product which might be considered to be a simple model for the starch iodine complex. Preparatory to an examination of the iodine complex, a brief crystallographic investigation was carried out on the uncomplexed dioxane. Inasmuch as the iodine complex appeared to be too unstable to permit the use of ordinary diffraction techniques, the study was discontinued.

Inspection of the molecular structure of 2,5-dimethoxy-2,5-dimethyl-1,4-dioxane indicates the possibility of *cis* and *trans* stereoisomers, and it was hoped that the determination of the crystal symmetry might distinguish between these possibilities. However, the monoclinic space group $C2/c$ with four molecules per cell requires only that the molecule must have either a center of symmetry (*trans*, chair form for the dioxane ring) or a two-fold axis (racemic mixture of *cis* forms; boat form for the dioxane ring).

Crystals of this compound are volatile; in the course of a few days' exposure to air the crystals were badly eroded although the diffraction patterns remained excellent. The unit-cell and space-group data were obtained by oscillation (Cu $K\alpha$) and Laue patterns:

$$a_0=11{\cdot}4,\ b_0=6{\cdot}4,\ c_0=13{\cdot}2\ \text{A.};\ \beta=95{\cdot}7^\circ;$$

space group Cc or $C2/c$ with four molecules per unit cell. These values are in fair agreement with optical crystallographic data given by Nef (1904)

$$(a:b:c=1{\cdot}77246:1:2{\cdot}00865,\ \beta=84^\circ\ 13',$$

monoclinic holohedral). The space group Cc may be eliminated assuming that the previous assignment to the monoclinic holohedral class is correct.

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